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A METHODOLOGY FOR THE SYNTHESIS OF COMPUTATIONAL MODELING AND EXPERIMENTAL DESIGN

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ABSTRACT

The development of new experiments focused on the analysis of different hazard characteristics of energetic materials can be expensive and time consuming. The progression of initial concepts into viable experiments that utilize available hardware can often be a tedious, trial and error process. However, coupling the experimental evolution with various available computational tools can lead to drastic savings in both time and money. The methodology for integrating computational modeling with experimental design is described in detail as a part of this paper. First, simple engineering analysis methods were used to determine the overall feasibility of initial concepts and designs. Once an initial concept is selected, an iterative process between the experimental design and high-fidelity computational models begins. The experimentalist establishes design boundaries and modeling is used to identify a variety of optimal configurations. This exchange between experimentalist and modeler occurs constantly during this phase of the design process. Much of this exchange is motivated by new limitations and requirements that emerge as a result of this synthesis. Ultimately, the design process is concluded when an optimal experimental design is identified and fabricated. The recent development of the controllable heat flux device utilized this synergetic relationship.

INTRODUCTION

With the advent of improved computational resources, a new suite of techniques has been provided to the hazard classification analysts, providing increased fidelity. However, traditional engineering calculations and analyses remain vital and useful parts of the research and design process. When engineering analyses and higher fidelity computational techniques are coupled with experienced experimental design, a dramatically improved design results. These improvements include an overall reduction in design and development time, reduced cost in both materials and labor, as well as the optimization of the final prototype.

The objective of this article is to detail a methodology used to couple various levels of analysis with experimental design and present a case study applicable to hazard classification efforts. At the heart of this effort is a small-scale test protocol intended to provide a valid alternate for the external fuel fire hazard classification test. The test case presented in this article will describe the development of a controllable heat flux device that plays an integral part in this alternate test initiative.

The methodology presented herein consists of 1) simple engineering analysis calculations, 2) iterative higher-fidelity design calculations, and 3) optimal performance prediction calculations. Further details describing this methodology will follow in the context of the case study.

CONTROLLABLE HEAT FLUX DEVICE CASE STUDY

In the bonfire test for hazard classification a test article can experience heat fluxes from 40 kW/m² to 400 kW/m², even at similar gas temperatures. Since the thermal response of energetic materials is dependent on both the incoming heat flux and temperature, it was desired to be able to better quantify

and control the incoming heat flux. A possible alternative was proposed and the concept idea is shown in Figure 1.

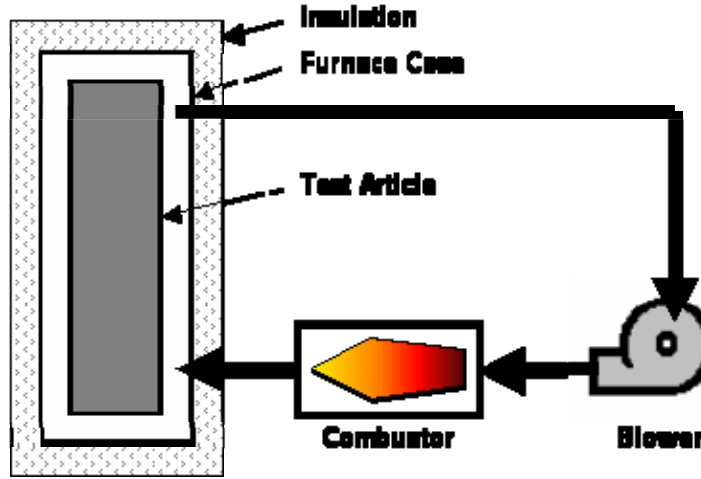


Figure 1. Initial Concept for Controllable Heat Flux Device.

One of the major tasks addressed by NAWCWD China Lake was the development of an experimental device that was capable of producing controllable and relatively high levels of heat flux for use with small-scale test samples. Computational tools were used at nearly every step of the design and construction in order to effectively allocate limited resources and provide an optimized overall design. A team was built consisting of experimentalists and computer modelers. The development of the controllable heat flux device from the concept to construction will be used as the case study to demonstrate the methodology in coupling experimental and computer modeling work to accomplish a desired task.

SIMPLE ENGINEERING ANALYSIS CALCULATIONS

Heat fluxes into objects submersed in pool fires range from 40 kW/m² to 400 kW/m². Using this range of heat fluxes, some simple calculations were performed to determine the feasibility of the proposed controllable heat flux device. The convective heat flux into the test article was estimated using Equations 1 - 3. [1]

$$q''_{conv} = h(T_{air} - T_{article}) \quad (1)$$

$$h = \frac{k}{D} Nu \quad (2)$$

$$Nu = 0.027 Re_D^{4/5} Pr_D^{1/3} \left(\frac{\mu}{\mu_s} \right)^{0.14} \quad (3)$$

Bounding calculations were done with various incoming gas temperatures (1000 K to 1500 K) and velocities (7.6 m/s to 91 m/s). Heat fluxes of 16 kW/m² to 170 kW/m² were calculated over the design space. These results were presented to the experimentalist. They commented that the temperature range was achievable. However, one of the constraints of the design was cost and portability. The desire was to provide the air with a relatively inexpensive fan and not use compressed air. They stipulated that the air mass flow rate should be around 0.45 kg/s and not exceed 0.90 kg/s. This corresponded with a velocity upper limit of ~27 m/s. This interchange with the experimentalist provided a more realistic upper bound for the convective heat transfer of 65 kW/m². The calculated heat flux at the desired mass flow of 0.45 kg/s ranged from 38 kW/m² to 20 kW/m² with air temperatures of 1500 K to 1000 K.

Realizing that radiation will be a major form of energy exchange in the device, simple bounding radiation heat flux calculations into the test article were performed. Equation 4 [1] was used to determine radiative heat flux exchange between concentric cylinders.

$$q_{rad}'' = \frac{\sigma(T_{wall}^4 - T_{article}^4)}{\frac{1}{\epsilon_{article}} + \frac{1 - \epsilon_{wall}}{\epsilon_{wall}} \left(\frac{D_{article}}{D_{wall}} \right)} \quad (4)$$

Stainless steel was the material to be used for the outer wall cylinder. The emissivity of hot stainless steel ranges from 0.5 to 0.8 depending on the level of oxidation. The emissivity of the test article could have a similar range for metal cases or higher for composite cases. Using the same temperature range for the outer wall as the hot incoming gas (1500 K to 1000 K) and wall emissivity of 0.65 and article emissivity of 0.8, the radiative heat flux was calculated to be 190 kW/m² to 30 kW/m². In the calculations using the low temperatures the contribution of radiation and convection to the heat flux into the test article are similar. Since the radiative heat flux is a function of the wall temperature to the fourth power, the contribution of radiation to the incoming heat flux increased much faster than that of convection. Using the upper temperature range, the radiative heat flux was calculated to be 5 times that of convection.

The initial heat flux calculations were important in that they showed that the device could deliver the desired heat flux to a test article. They also showed that there could be a significant amount of control of the heat flux into a test article by changing the incoming mass flow and temperature. These straightforward and easily performed calculations established feasibility and the design of the device was continued.

ITERATIVE HIGH-FIDELITY DESIGN CALCULATIONS

The simple engineering analysis effectively bounds and constrains the problem and allows an initial concept to be generated. The next step in the computational portion of the design process is the relaxation of the assumptions and generalities (geometry and physics) that are inherent in the simple engineering calculations. The added level of detail and improved accuracy provide necessary information in design of the actual design prototype. Numerical heat transfer methods were used to predict the response of the test article. Computational fluid dynamics (CFD) tools were used to estimate the flow and heat transfer around the test article within the combustor. Each of these areas will be discussed briefly.

NUMERICAL HEAT TRANSFER MODELING

During the initial phases of this project, NAWCWD China Lake created a transient thermal penetration model of a thermally protected composite-cased rocket motor. A two-dimensional axis-symmetric model was created using MPCoyote [2,3], a thermal analysis software package from Sandia National Laboratory. The model used temperature dependent properties for the primary materials and tracked the extent of thermal penetration as a function of time.

Figure 2 is a temperature versus time plot showing the thermal penetration of a composite cased rocket motor at a specified heat flux level. While this model neglected charring and ablation of the thermal protection layers and the graphite-epoxy composite case, it was useful in predicting the characteristic thermal profile and estimated the order of magnitude of the thermal penetration time. The experimentalist used the thermal penetration time information to determine the required size of the fuel source. The resulting thermal traces indicated a strong dependence on the thermal properties of the outer layers of the case system and showed that the appropriate physical mechanisms were required for these materials.

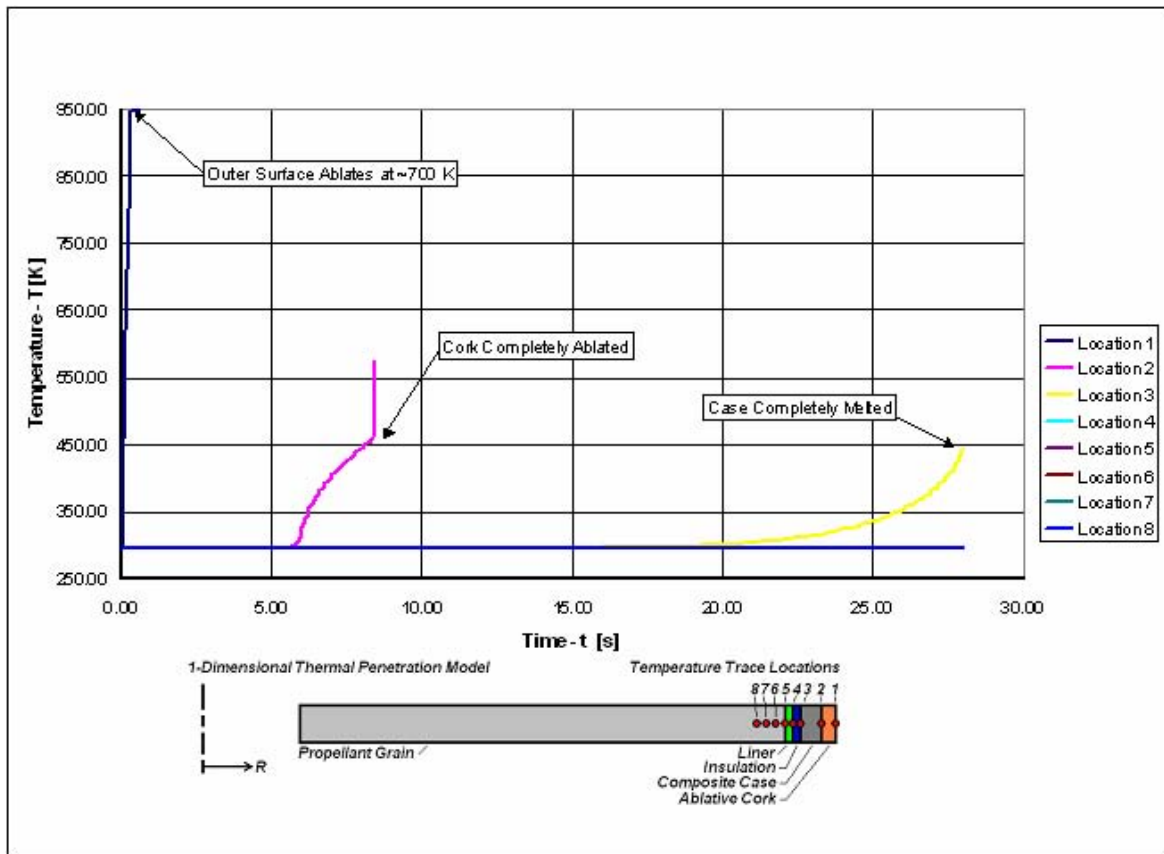


Figure 2. Temperature versus time profiles for a large diameter composite rocket motor exposed to an exterior surface heat flux of $q'' = 100,000 \text{ W/m}^2$.

It is necessary for any small-scale test article to represent the full-scale item as closely as possible. The experimental design of the small-scale article showed that when the thickness of the case wall (composite case, liner, and insulation) remained fixed and the overall diameter decreased, the test article case retained an excessive amount of strength. It was also unclear how the reduction in case thickness of the test article would affect the thermal response. These two competing system properties required detailed analysis and consideration. The detailed numerical heat transfer model was used to address the associated thermal issues.

The effect of the diameter of the propellant grain on the thermal penetration was analyzed using the numerical heat transfer model. To address this issue, the numerical heat transfer model of the full-scale rocket motor was compared to sub-scale analog models. The subscale models consisted of 0.454 m, 0.170 m, and 0.061 m diameter-propellant-grains motors. These subscale models employed the same thickness dimensions for the case materials, but varied the diameter of the propellant grain. Figure 3 displays the time dependent thermal traces of the full- and sub-scale models. The agreement of the curves in Figure 3 indicates that the predominant thermal effects occur in the case/insulation/liner materials and not in the propellant grain. From this result, it was concluded that a small-scale alternate test for the external fuel fire hazards classification test was feasible for large diameter, composite cased rocket motors.

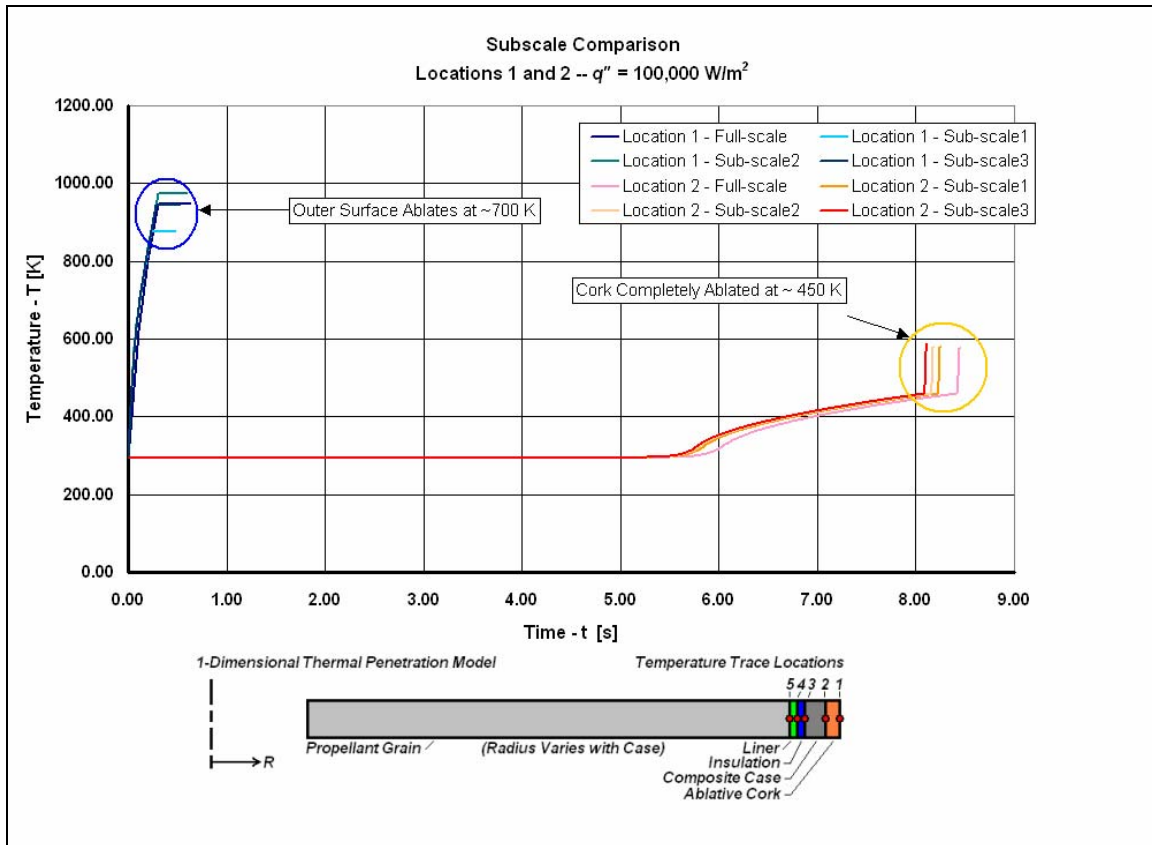


Figure 3. Thermal penetration profiles for full- and sub-scale motor models.

COMPUTATIONAL FLUID DYNAMICS SIMULATIONS

The engineering calculations of the heat flux into the test article gave bounding values, but higher fidelity calculations were desired to further refine the actual magnitude of the possible heat fluxes into the test article. The commercial CFD software Fluent [4] was used to determine the contribution of convection and radiation to the overall heat flux. The configuration used in the calculations is given in Figure 4.

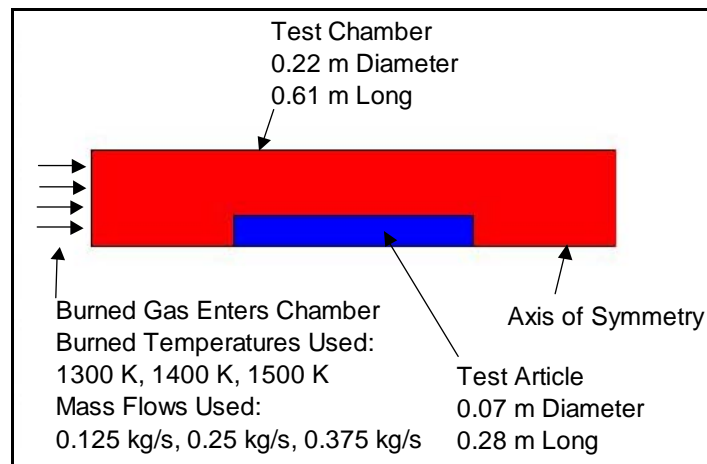


Figure 4. Computational setup for sizing calculations.

The calculations were done at two different test chamber diameters, three inlet gas temperatures, and three mass flows. The results are shown in Figure 5. The results demonstrated that the device could deliver almost an order of magnitude of different heat fluxes to the test article depending on the mass flow and the gas temperature. The results show that the radiative component of the incoming heat flux is the greatest.

It is important to note that the high fidelity calculation compare reasonable well with the simple engineering calculations. For the convective heat flux, the Fluent calculations and the simple equation calculations were within 25% - 50% of each other. This agreement between the separate calculations gives additional confidence to the results. The radiation calculations had the same trend, but the magnitude of the simple radiation calculation was up to 2 times that of the value calculated by Fluent. This was expected since the approximations were greatest for the simple radiative heat flux calculations and they were supposed to give an upper bound. This shows the importance of running the high fidelity calculations to refine the results.

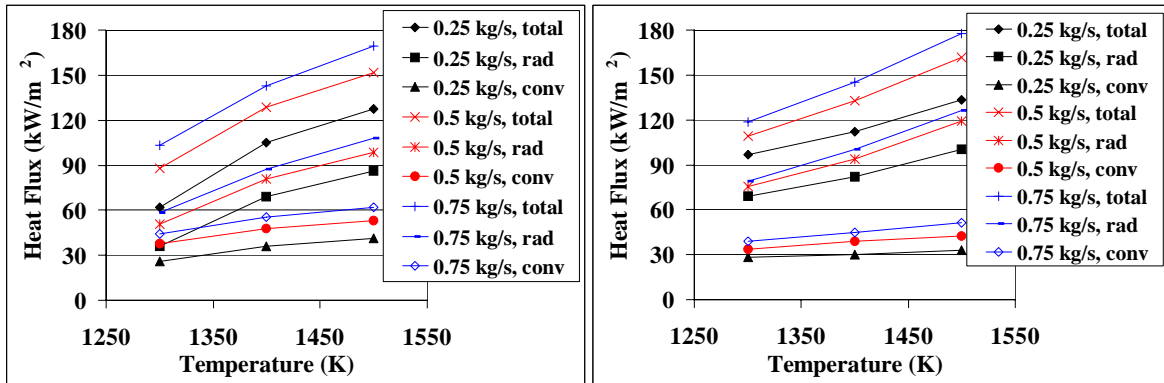


Figure 5. Heat Flux into Test Article vs. Temperature of Gas with a Chamber Diameter of 0.3 m (left graph) and 0.46 m (right graph).

Another advantage of high fidelity modeling is the additional information acquired. For overall heat flux, the simple and high fidelity model are comparable. However, the simple model gives no information on the flow structure or temperature distribution within the device. An example of the advantage of having this information is given in designing the fuel injectors. The experimentalist wanted to design the inlet diameter so the propane would sufficiently penetrate the chamber, but not cross the line of symmetry. It was suggested that 0.064 cm would work. Since the geometry and flow field were already in place, a drop model was added to investigate droplet dispersion. Figure 6 shows the propane droplet concentrations for injector openings of 0.25, 0.13, and 0.064 cm. The 0.25 cm diameter injector shown on the top did not penetrate enough of the test chamber, while the 0.064 cm diameter injector had too large of a penetration. The 0.13 cm diameter injector was chosen as the best option.

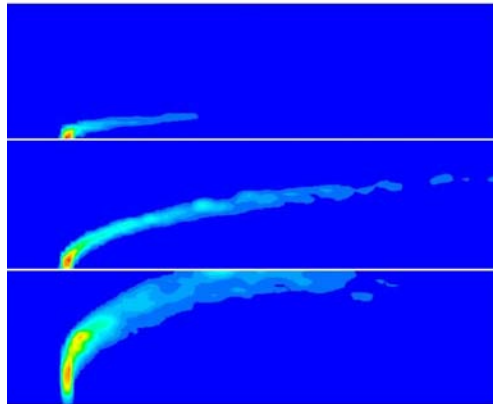


Figure 6. Droplet Concentration Profiles for Three Injector Diameters: 0.25 cm (top), 0.13 cm (middle), 0.064 cm (bottom).

OPTIMAL PERFORMANCE PREDICTION CALCULATIONS

The optimal design of the controllable heat flux device will require some amount of experimental trial and error. The device must be characterized and calibrated in order to provide meaningful results. For this purpose, a calibration tool is currently being designed and constructed. This device will use Heat Flux Microsensors (HFMs) to directly measure the total amount of heat flux applied to a cylindrical sample. HFM heat flux sensors were selected because they are capable of measuring radiant and cross flow convection heat flux simultaneously. The more commonly used Gardon gauges are not effective when exposed to high levels of cross flow convection.

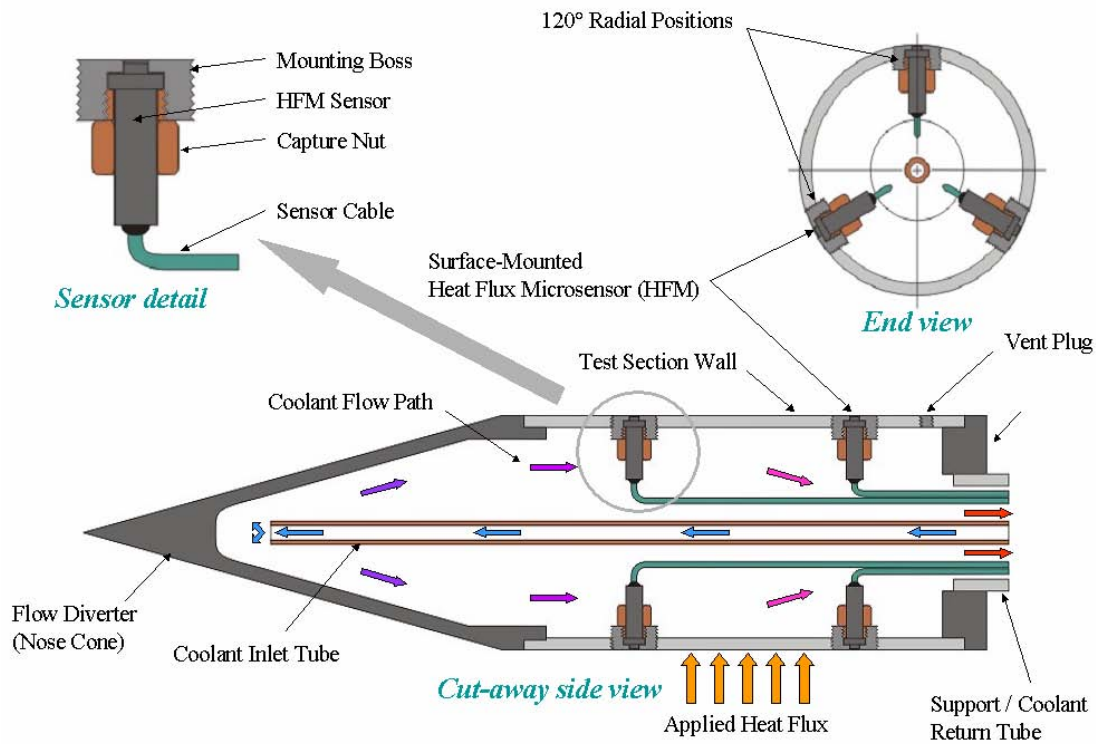


Figure 7. Conceptual design of the Heat Flux Calibration Device.

During the design of the calibration device, empirically based design calculations were performed to determine whether cooling of the device would be required. These calculations indicated that coolant water would indeed be required, but would be sufficient to maintain the HFMs at their required temperature. Figure 7 shows a conceptual design for the calibration device. It is expected that additional modeling will be required as the design of the calibration device is modified and optimized.

Additional CFD analysis was used in the design of the flow diverter nose cone. The cone was analyzed to minimize the flow separation off of the cone. Cone lengths of 8.9, 17.8, and 26.7 cm were used. It was determined that the 26.7 cm nose cone had the least flow separation and was not excessively long, so calculations were done with only a front nose cone. This was done to examine the configuration shown in Figure 7. The velocity profiles for the 8.9, 17.8, and 26.7 cm nose cones are shown in Figure 8 along with the profiles over the test article with only a front 26.7 cm nose cone.

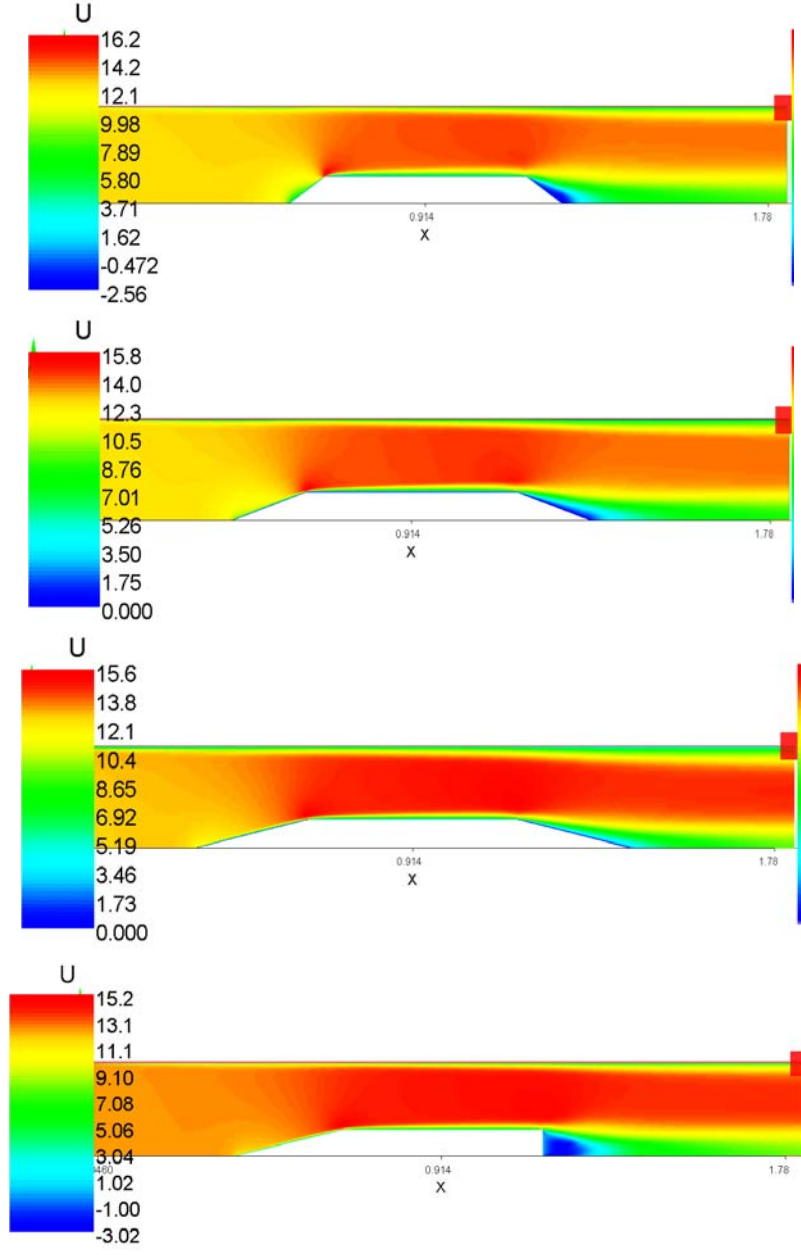


Figure 8. Velocity profiles with 8.9 cm (top), 17.8 cm (second from top), and 26.7 cm (second from bottom), nose cones and 26.7 cm (bottom) single front nose cone.

As the device is calibrated, the correct fuel and fan speed settings will be determined for the desired level of applied heat flux. A performance response function of the following form will be defined (illustrated here with three main effects and their interactions):

$$q''_{flux} = b_0 + b_1x_1 + b_2x_2 + b_3x_3 + b_{12}x_{12} + b_{13}x_{13} + b_{23}x_{23} + b_{123}x_{123} \quad (5)$$

using 2^k Factorial Experiments (Design of Experiments) techniques (see detailed descriptions of the methodology in [5,6,7]). Here b_i represent model coefficients determined during analysis, x_i represent primary effect variables, and x_{ij} and x_{ijk} represent the possible two- and three-way interactions of the main effect variables. These techniques aid in the identification of the significant and the insignificant parameters to the overall system performance. This type of analysis, while relatively simple to apply to this type of application, will provide a rigorous methodology to identify critical parameters and any

additional interactions between these parameters. Such interactions are often difficult to predict prior to actual testing and can aid in creating an optimized final design.

Once the Controllable Heat Flux Device prototype was designed and constructed, creation of a thermal model for the system response was initiated. Due to the thermal characteristics of the final design, both radiation from the heated flow tube and convection from the heated working fluid will be considered in order to predict the amount of heat flux applied to the small-scale sample. This model, while currently in development, will help to characterize the performance of the device during normal operating conditions.

RESULTS AND DISCUSSION

Synthesizing experimental design and computational modeling has traditionally been a challenge; however, using the methodology presented herein, several key results have been achieved. Most notably, the methodology as outlined was successful and can have positive results. Second, the method of synthesis has resulted in a working prototype of the controllable heat flux device. This prototype has achieved all of its stated objectives and was completed in an efficient and timely fashion. Finally, use of the method has resulted in a device capable of performing the tasks required by a sub-scale alternate test for the external fuel fire hazards classification test.

Several key lessons were learned during the case study described herein. First, the simulation cannot answer all the questions during the experimental design. Many aspects will require some trial and error with actual testing and this cannot be avoided. Direct experimental design and computational modeling should augment and assist each other at every step. They both have a place and provide added value. Second, computational results and models have limitations. These limitations are inherent in the simplifications and assumptions necessary to solve the fundamental equations that form the basis of the model. It is essential to know and recognize them so not to rely on incorrect or nonphysical results. Third, computational models should be used incrementally, starting from the simplest model that gives meaningful results. Complicated analysis should only be performed when added detail and accuracy are requisite for the experimental design. Therefore, computational analysis will not be needed at every stage of the design. Lastly, communication between the experimentalists and computationalists is vital at every step. The efforts cannot be performed independent of each other, but they must exchange constraints, information, and results continually.

SUMMARY AND CONCLUSIONS

A methodology for synthesis of experimental design and computational modeling was successfully implemented in the development of the Controllable Heat Flux Device. The methodology presented consists of 1) simple engineering analysis calculations, 2) iterative higher-fidelity design calculations, and 3) optimal performance prediction calculations. Computations will not replace direct experimental development, but should augment and enhance it. Communication is vital between experimentalist and computationalists to exchange constraints, information, and results continually.

FUTURE WORK

It is likely that computational efforts related to this project will continue to support design and fabrication activities. With the completion of the Calibration Device and an appropriate combustor thermal performance model, an assessment of the uniformity of the applied heat flux levels will be made. Computational methods will be the primary tools used in this assessment. It is likely that the characterization and performance of the device will be modeled during actual operation conditions for several test cases. Successful demonstration of the computational capabilities will open the door for future predictive modeling efforts.

ACKNOWLEDGMENTS

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